Torsion 12 [!#1;R2;r5:1]@[CX4;R1;r5:2]@;-[CX4;R1;r5:3]@[!#1;R2;r5:4] **Binned Counts** 0.12 Fit **ETKDG Fit** Probability per 10° Bin - 90.0 - 80.0 - - 10.0 - 10.0 - - 10.0 0.02 0.00 60 120 180 Torsion (°)